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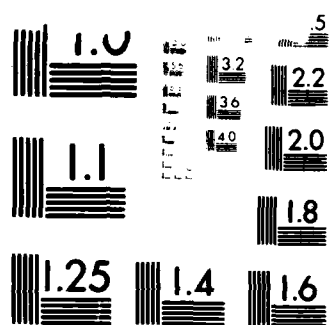
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Modern chemical instrumentation is capable of generating enormous amounts of data in very short periods of time. It is clear that a major task of scientists for the near future is to develop techniques to utilize more effectively this capability, in order to avoid the typical dilemma of being buried in data with little or no perspective of the information content. Thus, there are three key developments that must be pursued: definition of "information content"; identification of methods to correlate instrumental parameters with information content; and development of tools for the instrumental enhancement of information content and the efficient extraction of information from data. These developments should allow the evolution of "smart instruments", perhaps guided by artificial intelligence principles. This paper will describe some of the principles and tools that have already been developed, and will identify the areas where work needs to be done.

Modern instrumentation for chemical analysis, because of the incorporation of digital computer systems, allows the generation and collection of immense amounts of data. This is facilitated by computer

control of experimental variables and high-speed collection of multiple channels of data. This in turn allows complex measurement principles to be implemented, with correspondingly complicated multivariate analysis.

Unfortunately, the data explosion that has accompanied the evolution of modern chemical instrumentation has not provided a corresponding information explosion. This is because relatively little attention has been paid to the development of techniques for optimization of information content, or for enhancement and extraction of information. It is not uncommon to observe a scientist buried in a data printout from an experiment, manually scanning columns of data, calculator in hand, attempting to extract useful information.

It is time to turn our attention to developing more effective methods for obtaining information from complex experimental systems. The first step involves the definition of generic concepts of information content which are independent of the specific instrumental system. This is a task which has been surprisingly neglected in the past. The very simplest concepts which must be defined include:

- o informational goals
- o information content
- o information enhancement

The next step is to apply the basic principles of information theory, signal processing theory, multivariate data interpretation, and adaptive instrumental control in order to enhance and effectively extract information.

INFORMATION GOALS

The primary requirement in the process of information enhancement is

to define the informational goal(s) associated with a set of experimental measurements. Equally important is the definition of an appropriate measure of the degree to which the informational goal is achieved. Some generic qualitative informational goals and their respective figures of merit might be:

GOAL	FIGURES OF MERIT
concentration	accuracy/precision
resolution	peak separation/peak width
sensitivity	detection limit/response slope
matrix effects	linearity/interference effects

In addition, it is possible to define qualitative informational goals. These might include:

- o identification of chemical components
- o classification of materials/properties
- o establishment of chemical mechanism.

Corresponding figures of merit for the qualitative informational goals can be defined in terms of statistical accuracy by evaluation with systems of known properties.

INFORMATION CONTENT

This concept is one of the most difficult to quantitate. There are some relatively explicit definitions of information content for electronic communications. (For example, the Nyquist theorem defines the minimum sampling rate required in order to preserve the maximum frequency information in a periodic signal. And, the relationships between digital encoding formats and information content of a data base can be

quantitated.) However, for the general problem of evaluating the results of instrumental measurements of chemical systems, the definitions for information content of data are very clear.

One goal of our research program is to develop explicit and quantitative definitions of information content which may be useful for chemical instrumentation systems. These will be based on the principles of information theory, sampling theory, and signal processing theory. At this time, however, we can describe an empirical approach to evaluation of information content which we have found very useful.

This approach involves the following steps:

- o define the "desired information" (informational goal(s))
- o define a figure of merit for goal achievement (e.g., accuracy, precision, reliability, etc.)
- o empirically determine "information content" from the relationship:

$$[\text{INFO. GOAL}] = f[\text{INFO. CONTENT}] \quad (1)$$

From the above statement the information content of a chemical measurement system can be evaluated by studying the effects of experimental factors on the degree of achievement of the informational goal(s). This is elaborated below.

INFORMATION ENHANCEMENT

An empirical procedure can be defined for the enhancement of information content. First, it must be recognized that the achievement of desired informational goal(s) depends not only on the inherent

information content of data, but also on the data management and analysis procedures. This is expressed in Equation (2):

$$[\text{INFO. GOAL}] = f[\text{CONTENT, MGHT, ANALYSIS}] \quad (2)$$

Thus, to examine the relationship between information content and experimental factors, it is necessary to maintain consistent data management and analysis procedures. Then, one can assume a direct relationship between the achievement of informational goals and information content as implied in Equation (1).

A study designed to determine the effects of experimental factors on information content might be based on the relationship defined by Equation (3):

$$[\text{INFO. CONTENT}] = f[\text{MEASUREMENT PRINCIPLES,} \\ \text{EXPTL DESIGN,} \\ \text{EXPTL PARAMETERS}] \quad (3)$$

Procedurally, one could vary any of the experimental factors in Equation (3) and evaluate the effects on information content under conditions where Equation (1) applies.

In order to clarify the general concepts defined in the above sections, the following sections will describe an experimental study which followed those principles in order to achieve specified informational goals.

ELECTROCHEMICAL STRUCTURAL AND ACTIVITY CLASSIFICATIONS

The classification of chemical structure using electrochemical techniques, is a challenging problem. Voltammetric responses lack fine structure and probably will never compete with spectroscopic methods in qualitative analysis. The complex dependence of an electrochemical response on many variables, and theoretical problems in relating structure to electrochemical activity, make qualitative voltammetric analysis even more formidable.

Even though the difficulties in qualitative electroanalysis are great, the rewards of developing a reliable means of structural identification through electroanalysis would also be great. Due to recently developed miniaturization techniques, electrodes are the most promising probes of in vivo chemical species. Carbon fiber electrodes may be implanted within a single cell or neuron (1). Electrochemical detectors in liquid chromatography are becoming very important because of their high sensitivity and selectivity. Quantities of electroactive material in the picogram range have been analyzed. Osteryoung, et al. (2) have demonstrated the feasibility of scanning the potential of a liquid chromatographic electrochemical detector, so the development of qualitative voltammetric methods ~~would open up the possibility~~ of the characterization of eluants that are 1000 times less concentrated than those which can be analyzed by spectroscopic techniques.

Linear-free-energy relationships have generally been the most useful expressions for relating structure to electrochemical activity in the past. A substituent group will have a characteristic effect on the free energy of an electrochemical reaction occurring in its vicinity. This effect may occur through electron withdrawal, electron donation, or it

may be steric in nature. In any case, the effect may be quantified through the use of Hammett substituent constants. For a given class of electrochemical reactions, there will be a linear relationship between $E_{1/2}$ and the substituent constants σ (3).

There are two main problems in the use of linear-free-energy relationships. The first and largest problem is the determination of the reaction series to which an unknown belongs. Such a deduction from electrochemical behavior is not straightforward. Furthermore, there may be several reaction series which may be constructed for a class of compounds depending on solution conditions. The slope of the $E_{1/2}$ vs σ plot would be different at high pH's due to a change in the mechanism of reduction.

The second main problem is that there is often not enough $E_{1/2}$ separation for different substituents or substituent combinations to allow for confidence in identification, especially when experimental reproducibility is low due to uncontrolled matrix effects. The consideration of more information than $E_{1/2}$ would clearly be helpful.

Because pattern recognition is well suited to the consideration of large amounts of information and to making use of obscure relations, we have applied it to chemical structure identification from electrochemical data. The main questions have been what data should be collected and how much?

Burgard and Perone (4), used staircase voltammetry to analyze 29 compounds belonging to four different electroactive group/skeleton combinations. The classes examined were aromatic-nitro, aliphatic-nitro, aromatic-aldehyde and aromatic-aliphatic-ketone. Fortunately these classes were almost completely separated on the basis of peak potential;

but this feature alone cannot be considered sufficient for many identification problems. Thus, the voltammograms were examined for any shape information which might characterize a particular electroactive group or the skeleton to which it was attached. It was found that the change in peak shape with scan rate produced fair classifications (70% correct), but that complete separation of the classes was not possible for the experimental conditions and compounds which were chosen. The results suggested that the information content of the electrochemical data base should be increased for more reliable structural classifications.

The work described below by Byers, Freiser, and Perone (5,6) represents an attempt to define quantitatively the information content of electroanalytical voltammetric data with regard to structural and activity classifications. The general principles defined in the introductory sections of this paper were followed.

RESULTS AND DISCUSSION

Ichise, Yamagishi and Kojima (7-9) have proposed the simultaneous determination of complete E-i-c and C_{dl} -E-c patterns (c = surface concentration) and have published several papers on instrumentation and data compression algorithms for reaching that goal. E-i-c patterns were generated by applying a pseudo-random waveform to the cell and monitoring the current response. The surface concentration of the depolarizer was calculated from the current in an analog fashion with an " $s^{-1/2}$ module" which eliminated the effect of diffusion. C_{dl} was obtained by applying a high frequency 10 mV sinusoidal wave to the cell and measuring the amplitude of the 90 degrees out-of-phase component of the current.

The idea of obtaining double-layer capacity information may be fruitful. The capacitance of the double layer is dependent on adsorption of the analyte, and the strength and potential dependence of adsorption may indicate the presence of certain functional groups (10).

π -electron interaction between adsorbed molecules and the electrode surface has a characteristic influence on the adsorption behavior of organic substances (10), and specific interactions between the analyte and some other molecule or ion within the double layer may also be helpful in identification (11,12). Some adsorbed organics will inhibit the reduction of metal ions, while others, through the so called "cap-pair" effect will accelerate reductions (13).

The use of a potential-step technique such as cyclic staircase voltammetry represents a simple alternative to Ichise's method (8) of obtaining information on both adsorption and electron transfer kinetics. The current decay immediately after a step is primarily capacitive while current at later times is almost totally due to electron transfer reactions. Thus, by measuring the current at several times during each step and by changing the scan rate, information on both the kinetics of the electrode process and the differential capacity can be obtained with a single sweep.

As is true with cyclic linear sweep voltammetry, the reversal of the scan is important in detecting chemical reactions which succeed the electron transfer step. Immediate repetition of a cyclic scan may detect products which have been generated in the reverse scan of the first cycle.

One additional parameter which can be explored is the "drop hang time". This refers to the time period between the creation of a stationary mercury drop and the beginning of the first staircase scan.

During the waiting time, a potential can be applied. This variable was investigated in our work to see if there was any class specific information in the kinetics of adsorption.

Another source of structural information is the electrochemical response of the analyte to chemical perturbations. Changes in solution conditions have been useful in classical studies of structure-activity relationships. Exploration of a variety of solutions will help define the best conditions for particular classification problems.

All of the experimental and solution variables which have been examined systematically in our classification studies are listed in Table 1. The determination of the effect of each of the seven variables is difficult without good experimental design. To characterize all main effects and all interactions one could arrange the experiments by a factorial design (14). For the seven variables considered here, 128 runs would be needed for each compound. The large number of runs can be avoided by using a saturated fractional factorial design (15) in which the main effect of all seven variables can be investigated in only eight experiments. By running a second fraction, in which all variable levels have been reversed from their state in the first fraction, all confounding between the main effect of variables and the interaction of two variables will be eliminated. Higher order interactions (the interaction of three or more variables) may still be confounded with the main effects, but in most cases such interactions are relatively small in magnitude.

In our work (5,6), a fractional factorial design was used as described above. In addition, one of the experiments run early in the analysis of each compound is repeated near the end of the analysis to

TABLE 1. Variable levels for factorial design to study structural effects on voltammetric data.

VARIABLE NUMBER	VARIABLE	LOW LEVEL (-)	HIGH LEVEL (+)
X ₁	% Ethanol	0.5 %	9.5 %
X ₂	pH	8.0	5.1
X ₃	Surfactant Concentration	0	1.4×10^{-5} M
X ₄	Number of Cycles	1	2
X ₅	Scan Rate	0.25 V/s.	1.0 V/s.
X ₆	Drop hang Time	0.2 s.	30 s.
X ₇	Sampling Time	30% of step ($\alpha'=.7$)	end of step ($\alpha'=.007$)

determine instrumental precision and to detect any decomposition of the sample. This makes a total of 17 voltammograms which must be taken for each compound. These experiments yield 17 current-voltage and 17 differential capacity curves for each compound.

Graphical analysis of the error involved in the calculation of variable effects was done for several nitroaromatics and nitrophenyl ethers (5). It was discovered that all of the variables chosen for study had significant effects on the Faradaic responses of the compounds examined. The magnitudes of the effects and the shapes of the effect curves were quite different, indicating that redundant information was not recorded. All of the variables also had a significant effect on the differential capacity curves of strongly adsorbed species, but some of the effects could not be distinguished from noise for more weakly adsorbed compounds. Only pH, number of cycles and % ethanol had a significant effect on the capacitance response of both weakly and strongly adsorbed organics.

Since the variables chosen and the levels over which they were changed seemed to be appropriate for most compounds from a signal-to-noise perspective, the variable effects were further examined for any information which might be useful in structural classifications. Forty-five compounds representing three major structural classes were chosen, and features derived from the variable effects were tested for predictive ability (6). Class 1 consisted of 19 nitroaromatics containing a single benzene ring; Class 2 contained nine nitrodiphenylethers, and Class 3 consisted of 17 azo compounds. The classes were completely overlapped in potential, and all compounds were reduced by the same number of electrons, so the identification of the classes from their voltammetric behavior was not a trivial problem.

In terms of the concepts defined in the introductory sections, the informational goal of this study was "structural classification". The figure of merit for achievement of this goal was "classification accuracy" for examination of a data base containing a large number of items of known class. The experimental parameters were varied systematically according to a fractional factorial design. Ultimately, it was desired to establish what combination(s) of experimental parameters produced electroanalytical data with the highest information content, using the figure of merit defined above.

The pattern recognition analysis revealed that all of the variables produced structural-specific information. Most of the information was found in the Faradaic responses. Changes in the Faradaic responses with the number of cycles gave the highest classification accuracy of 93.3%. Scan rate changes yielded 89%, while pH, surfactant and drop hang time all produced classification accuracies of 84%. Changes in Faradaic response with % ethanol and sampling time appeared to contain the least structural information, giving classification accuracies of 66.7 and 75.6%, respectively. As was expected from the signal-to-noise analysis, the effects of the several variables on the capacitive responses were much poorer structural predictors. Classification accuracies ranged between 60.0 and 75.6%.

Although changes in differential capacity responses caused by changes in the experimental variables were not very helpful, the shapes of differential capacity curves which were obtained under the same experimental conditions were excellent structural descriptors. Using shape features derived from differential capacity curves taken under one set of experimental conditions, 93.3% classification accuracy was

achieved. Four other sets of experimental conditions yielded over 90% classification accuracy.

An interesting sidelight of the organic structural classification study was that herbicidal activity could also be predicted (6). The nitrodiphenylethers could be divided into compounds which were strong herbicides and those compounds which showed little or no herbicidal activity. Both Faradaic and capacitive responses could be used to separate these classes for over half the experimental conditions examined. As was found in the classification of structure, capacitive factorial features performed somewhat better than Faradaic factorial features. It also appeared that classifications of herbicidal activity using Faradaic factorial features could be improved considerably by working at high pH and without surfactant present. The information content of Faradaic or capacitive variable effects data could be improved by variations in % ethanol.

The ability of voltammetric responses to predict the herbicidal activity can be explained by the mechanism of herbicidal action for the nitrodiphenylethers. It is thought that these compounds are involved in the initiation of destructive free radical reactions with the phospholipid molecules which make up cellular membranes (16). Since the first step in the reduction of aromatics at the mercury electrode also involves the formation of radical species (17), some correlation between herbicidal activity and voltammetric behavior is not surprising.

CONCLUSIONS

The experimental study described here illustrates how the application of the principles of information enhancement can significantly improve

chemical analysis. In this case we have established the optimum conditions for obtaining structural or activity information from voltammetric electroanalytical data. Moreover, it is clear that the informational goal(s) will dictate the most favorable choice of experimental conditions. It is also interesting to observe that the most useful experimental conditions --- such as the enhancement of surface interactions --- are not necessarily those which are traditionally valued most highly in voltammetric studies. This result points up another valuable benefit of an objective systematic information enhancement study. Finally, it should be observed that the principles and general methodology described in this work are generic and should be applicable to any chemical instrumental systems.

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